

Nonlinear Surface Impurity in a Semi-infinite Lattice

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Abstract

We examine the formation of bound states on a generalized nonlinear impurity located at or near the beginning (surface) of a linear, tight-binding semi-infinite lattice. Using the formalism of lattice Green functions, we obtain in closed form the number of bound states as well as their energies and probability profiles, for different nonlinearity parameter values and nonlinearity exponents, at different distances from the surface. It is shown that close to the surface, the amount of nonlinearity needed to create a bound state or to effect dynamical selftrapping, increases (decreases) depending on whether the exponent is smaller (larger) than, approximately, two.

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The interplay of nonlinearity and discreteness has received considerable attention recently[1], since it plays a vital role in the emergence of a new kind of excitation in extended, nonlinear systems with discrete translational invariance, known as intrinsic localized modes (ILM). These ILMs are generic to physical systems of interest, such as arrays of nonlinear optical waveguides[2], molecular crystals[3], biopolymers[4], arrays of Josephson junctions[5] and even Bose-Einstein condensates in magneto-optical traps[6].

Given the strictly local manner in which nonlinearity enters into the effective evolution equations in all these cases (see below), one is led to the idea that in the limit of strong nonlinearity, one could approximate a typical nonlinear system by a linear one containing a small cluster of nonlinear sites, or even a single nonlinear impurity. The system thus simplified is amenable to exact mathematical treatment, and the influence of other, potentially competing effects such as dimensionality, boundary effects, noise, etc., can be more easily studied without losing the essential physics.

For a one-dimensional discrete system in the presence of a single nonlinear impurity, located at $n = d$, the dynamics is given by the well-known discrete nonlinear Schrödinger (DNLS) equation:

$$i\frac{dC_n}{dt} = V(C_{n+1} + C_{n-1}) - \chi|C_n|^\beta C_n \delta_{n,d}, \quad (\hbar \equiv 1) \quad (1)$$

where C_n is the probability amplitude for finding the excitation on site n , V is the nearest-neighbor transfer matrix element, χ is the nonlinearity parameter and β is the nonlinearity exponent. Usually, but not always, $\beta = 2$ which in a condensed mater context corresponds to an underlying harmonic oscillator degree of freedom ‘enslaved’ to the excitation (electron) at the impurity site. When this vibrational impurity is anharmonic in nature, other β values are possible in principle, with $\beta < 2$ corresponding to a “hard” vibrational impurity while $\beta > 2$ corresponds to a “soft” case[7].

Bound states for single nonlinear impurities embedded in infinite lattices include chains[10, 11, 12], Cayley trees[14], triangular[16] and a cubic[15, 16] lattices. Now, since the creation of a bound state, or the dynamical selftrapping at the impurity site implies the localization of energy on a scale of the order of the lattice spacing, one might surmise that, by placing the nonlinear impurity at or near the surface of a semi-infinite lattice, the nonlinearity strength needed to effect localization would decrease, facilitating in this way its creation and experimental observation. As an step in that direction, in this work we exam-

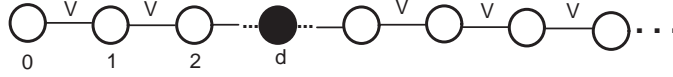


FIG. 1: A nonlinear impurity near the surface of a one dimensional chain

ine a simple model consisting of an electron (or excitation) propagating in a semi-infinite, linear chain, that contains a single nonlinear impurity at a distance d from the beginning ('surface') of a semi-infinite chain (Fig. 1), and examine the conditions for the existence of bound state(s) and the dynamical selftrapping properties, and compare them to the results obtained for the infinite chain [11].

Bound States. We consider Eq.(1) for a semi-infinite lattice ($n = 0, 1, \dots$) and normalize all energies to the half bandwidth of the infinite chain case. The Hamiltonian is given by

$$H = \frac{1}{2} \sum_{n=0}^{\infty} (|n\rangle\langle n+1| + |n+1\rangle\langle n|) + \gamma |C_d|^\beta |d\rangle\langle d| \quad (2)$$

where $\{|n\rangle\}$ are Wannier states and $\gamma \equiv \chi/(2V)$. The dimensionless Green function $G = 1/(z - H)$ can be formally expanded as[18] $G = G^{(0)} + G^{(0)}H_1G^{(0)} + G^{(0)}H_1G^{(0)}H_1G^{(0)} + \dots$, where $G^{(0)}$ is the unperturbed ($\gamma = 0$) Green function and $H_1 = \gamma |C_d|^\beta |d\rangle\langle d|$. The series can be resumed to all orders to yield

$$G_{mn} = G_{mn}^{(0)} + \frac{\gamma |C_d|^\beta G_{md}^{(0)} G_{dn}^{(0)}}{1 - \gamma |C_d|^\beta G_{dd}^{(0)}}. \quad (3)$$

where $G_{mn} \equiv \langle m|G|n\rangle$. Now, we cannot use Eq.(3) directly since we do not know C_d , but we will determine it through an exact selfconsistent procedure: The energy of the bound state(s) is obtained form the poles of G_{mn} , i.e., by solving $1 = \gamma |C_d|^\beta G_{dd}^{(0)}(z_b)$. On the other hand, the bound state amplitudes C_n are obtained form the residues of G_{mn} at $z = z_b$. In particular, at the impurity site, $|C_d|^2 = \text{Res}\{G_{dd}(z)\}_{z=z_b} = -G_{dd}^{(0)2}(z_b)/G_{dd}^{(0)'}(z_b)$ Inserting this back into the bound state energy equation leads to

$$\frac{1}{\gamma} = \frac{G_{dd}^{(0)\beta+1}(z_b)}{[-G_{dd}^{(0)'}(z_b)]^{\beta/2}}. \quad (4)$$

The unperturbed Green function $G_{mn}^{(0)}$ for the semi-infinite lattice, can be calculated by the method of mirror images: Since there is no lattice to the left of $n = 0$, $G_{mn}^{(0)}$ should vanish identically at $n = -1$. Thus, $G_{mn}^{(0)}(z) = G_{mn}^\infty(z) - G_{m,-n-2}^\infty(z)$, where $G_{mn}^\infty(z)$ is the Green

function for the infinite lattice, $G_{mn}^\infty(z) = \text{sgn}(z)(1/\sqrt{z^2-1})[z - \text{sgn}(z)\sqrt{z^2-1}]^{|n-m|}$, where $\text{sgn}(z) = +1(-1)$ for $z > 0(< 0)$. Therefore,

$$G_{mn}^{(0)}(z) = \text{sgn}(z) \frac{1}{\sqrt{z^2-1}} [z - \text{sgn}(z)\sqrt{z^2-1}]^{|n-m|} - \text{sgn}(z) \frac{1}{\sqrt{z^2-1}} [z - \text{sgn}(z)\sqrt{z^2-1}]^{|n+2+m|}. \quad (5)$$

From Eq.(5) we note the parity property $G_{dd}^{(0)}(-z) = -G_{dd}^{(0)}(z)$, which implies $G_{dd}'^{(0)}(-z) = G_{dd}'^{(0)}(z)$. This means, according to Eq.(4) that the change $\gamma \rightarrow -\gamma$, reverses the sign of z_b . On the other hand, from Eq.(1), it is possible to deduce that the change $\gamma \rightarrow -\gamma$ is equivalent to the change $C_n \rightarrow (-1)^n C_n^*$. Since we are interested in a localized state, where the C_n can be chosen as real, we conclude that a change in sign of the nonlinearity parameter reverses both the “staggered” character of the bound state and the sign of the localized state energy.

After inserting Eq.(5) into (4), the general structure for the number of bound states emerges: For any finite distance d from the surface and any positive value of the exponent β , there is a critical amount of nonlinearity γ below which there is no bound state, and above which there are two bound states. For β exponents smaller than 2, and as d is increased, one of the bound states tends to merge with the band edge, so that in the limit of a very deep impurity, there is only a single localized bound state. For $\beta > 2$, however, as d is increased, both bound states remain localized. In the special case of a linear impurity ($\beta = 0$), there is a single bound state provided $\gamma > 1/(d+1)$. Thus, in the limit $d \rightarrow \infty$ these results are consistent with the case of a completely infinite lattice[11]: A single bound state for $\beta < 2$, and for $\beta > 2$, a critical curve in nonlinearity strength-nonlinearity exponent space, separating a region with no bound states from a region with two bound states. At the surface ($d = 0$) the critical curve is given by

$$\gamma_c = \frac{(1+\beta)^{(1+\beta)/2}}{2\beta^{\beta/2}} \quad (6)$$

In particular, for the DNLS case, $\gamma_c = 3^{3/2}/4 \approx 1.3$, larger than the value for the infinite chain ($\gamma_c = 1$). Figure 2 shows phase diagrams in γ - β space showing the number of bound states, at different distances d between the impurity and the ‘surface’ of the system.

As to the stability of these bound states, it is easy to see from a graphical analysis of the structure of Eq.(4) that, as nonlinearity γ is increased one of the bound states becomes

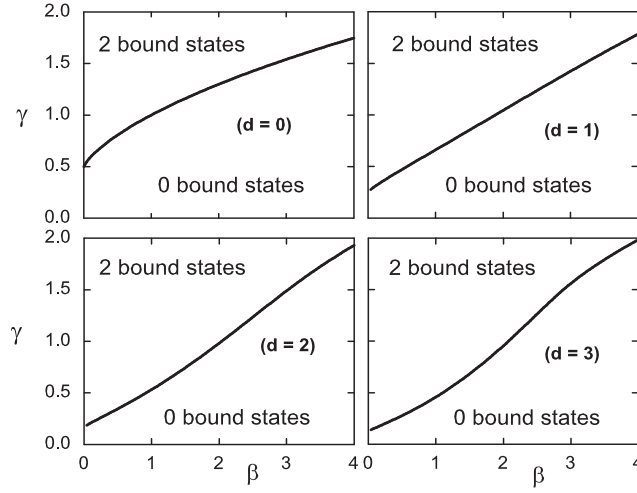


FIG. 2: Phase diagram in γ - β space, showing the number of bound states, for different distances impurity-surface (in units of the lattice constant).

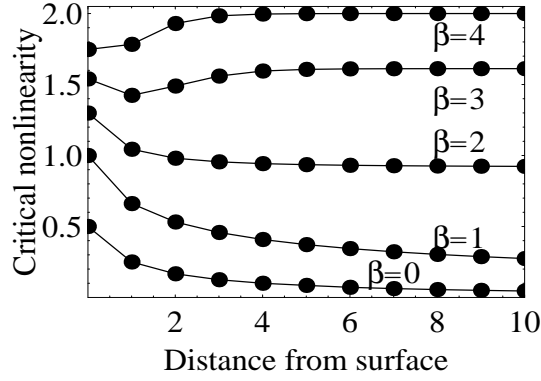


FIG. 3: Scaled critical nonlinearity for onset of a bound state, as a function of the distance from the nonlinear impurity to the ‘surface’ of the chain.

more and more localized, while the other becomes more and more delocalized. Since, in the limit of high nonlinearity, the effective coupling among sites is negligible, one would expect the bound state to become more and more localized. Therefore, the state with smaller localization length is stable, the other unstable. This qualitative argument is confirmed by the more rigorous procedure of examining the Hamiltonian flow of the system around the two fixed points (bound states).

Figure 3 shows the critical nonlinearity for the onset of a bound state, as a function of the distance from the impurity to the lattice ‘surface’ ($n = 0$), for different nonlinearity ex-

ponents. Significant differences from the infinite lattice case are apparent: As the impurity is placed closer and closer to the surface, the critical nonlinearity to create a bound state increases or decreases, depending upon whether the nonlinear exponent is below or above, approximately two. In particular, for the all-important standard DNLS case, $\beta = 2$, the presence of a surface increases the nonlinearity needed to create a bound state, contrary to popular belief that a surface would help localize the electron.

For a given value of exponent β and any inclusion distance d , the bound state probability profile $|C_n|^2$ is given in closed form by $|C_n|^2 = A[Q^{|n-d|} - Q^{|n+d+2|}]$, where $Q \equiv z_b - \sqrt{z_b^2 - 1}$, $A \equiv (z_b - Q)/(z_b + (z_b + 2(1+d)\sqrt{z_b^2 - 1})Q^{2(1+d)})$ and z_b is the solution of Eq.(4). Simple analysis of this profile shows that $|C_n|^2$ has always a single hump at $n = d$. This profile is shown in Fig.4 for the standard DNLS ($\beta = 2$) and a nonlinearity strength γ just above critical, at four different impurity locations under the surface. its general features are shared by other β exponents. Below the surface, the probability profile converges quickly to the

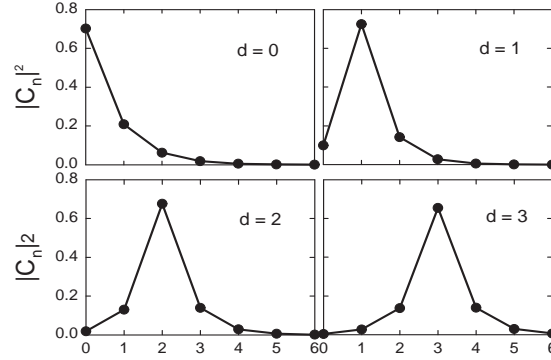


FIG. 4: Probability profile for the stable bound state at different impurity positions ($\beta = 2$, $\gamma = 1.305$).

infinite lattice case as d increases past 4.

Dynamical Seltrapping. We compute numerically the long-time average probability at the impurity site, $P_d = \lim_{T \rightarrow \infty} (1/T) \int_0^T dt |C_d|^2$, for several distances d from the ‘surface’ ($n = 0$). As initial condition, we use a completely localized excitation on the impurity site: $C_n(0) = \delta_{nd}$. Figure 5 shows the critical nonlinearity for selftrapping ($P_d > 0$) as a function of the distance between the nonlinear impurity and the chain surface, for different nonlinearity exponent values. In general, the behavior is qualitatively similar to the one observed for the onset of a bound state (Fig.3). In both cases, for a fixed distance, an

increase of the nonlinear exponent β results on an increase of the nonlinearity threshold for selftrapping. The same behavior was observed previously for an impurity in a completely infinite chain[11]. This phenomenon is not hard to explain: Since $|C_n| < 1$, we see from Eq.(1) that as $\beta > 0$ is increased, $|C_d|^\beta$ will necessarily decrease, which implies that a larger γ will be needed to keep the value of the *effective* impurity strength $\gamma|C_d|^\beta$. Thus, at a fixed impurity-surface distance, a higher β implies a higher γ_c . Another interesting behavior we observe from figs.5 and 3 is that for a fixed nonlinearity exponent, the critical nonlinearity depends roughly on whether the exponent is below or above two, approximately: For $\beta < 2$, an increase in the impurity-surface distance d results on a decrease of γ_c , while for $\beta > 2$, an increase in d increases γ_c . The explanation of this phenomenon seems to rest on the delicate balance between kinetic and potential energies. If we assume an electronic bound state Ψ with localization length λ , then on normalization grounds we have $|\Psi|^2 \sim 1/\lambda$. The kinetic energy content is $\Delta K \sim \hbar^2/2m\lambda^2$, while the average potential energy is in magnitude equal to $\Delta V = \int dx V(x)|\Psi(x)|^2 = \int dx \gamma|\Psi(x)|^\beta|\Psi(x)|^2 \sim \gamma a/\lambda^{1+(\beta/2)}$, where a is of the order of the lattice spacing. Thus,

$$\Delta V/\Delta K \sim \gamma \lambda^{1-(\beta/2)}. \quad (7)$$

On the other hand, as the impurity is brought closer to the surface, the wavefunction becomes more ‘compressed’ (Fig.4), i.e., λ decreases as d approaches zero. This implies, from Eq.(7) that for $\beta > 2$, a decrease in λ increases ΔV with respect to ΔK , which means that less nonlinearity is needed to maintain a localized state. On the contrary, if $\beta < 2$, an decrease in λ decreases ΔV with respect to ΔK and now, more nonlinearity is needed to maintain the localized state.

Completely nonlinear lattice. In the large nonlinearity limit where $\gamma \gg \gamma_{cr}$, the single nonlinear impurity results should approximate those corresponding to a whole nonlinear lattice. For the particular case examined in this work, the “extended” problem consists of the formation of an intrinsic localized mode (ILM) in a semi-infinite nonlinear lattice. Due to the presence of a surface, the discrete translational invariance is broken and a natural question arises: where will the localized state be formed? Our single nonlinear impurity analog can provide an answer. For each impurity position d , the bound state energy can be computed as a function of d . The position corresponding to its minimum value will correspond to the position of the ILM. Also, the impurity energy and spatial probability profile should approximate the ones corresponding to the ILM. Figure 6 shows the impurity

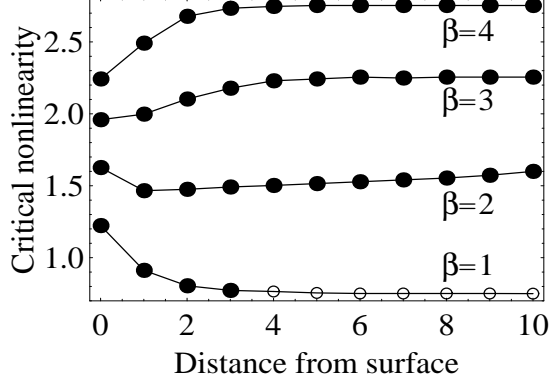


FIG. 5: Right: Scaled critical nonlinearity for dynamical selftrapping as a function of the distance from the impurity to the chain surface, for several nonlinearity exponents. The empty circles shown for $\beta = 1$ and $d = 4$ through $d = 10$ indicate approximate values since the selftrapping is not abrupt.

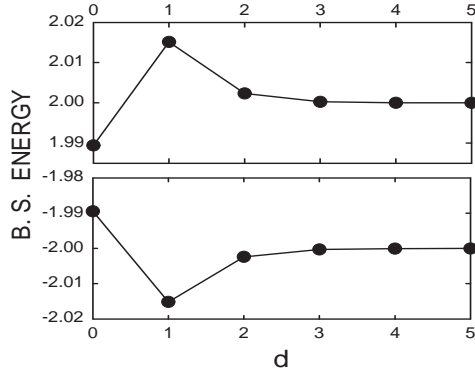


FIG. 6: Nonlinear impurity bound state energy as a function of distance impurity-surface, for $\beta = 2$ and $\gamma = 2$ (upper) and $\gamma = -2$ (lower).

energies as a function of distance from the lattice surface, for the DNLS case, $\beta = 2$ and $\gamma = \pm 2$. We see that for a positive value of the nonlinearity parameter γ , the preferred position is the very surface ($d = 0$), while for a negative γ , the preferred position is one layer below the surface ($d = 1$). These predictions are indeed confirmed by direct numerical computations, where the Hamiltonian corresponding to a semi-infinite nonlinear lattice $H = (1/2) \sum_{n=0}^{\infty} (|n\rangle\langle n+1| + |n+1\rangle\langle n|) + \gamma \sum_{n=0}^{\infty} |C_n|^\beta |n\rangle\langle n|$, is diagonalized by an iterative procedure. For the particular example of fig. 6, the error obtained for the ILM energy is about 1%.

Acknowledgements

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